

Print selected from 10565446_Rxn2.trn

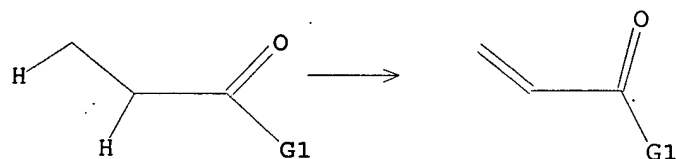
Uploading C:\Documents and Settings\dodell1\Desktop\10565446_Rxn7.str

L4 STRUCTURE UPLOADED

=> D L4

L4 HAS NO ANSWERS

L4 STR



G1 O,S,N,P

Structure attributes must be viewed using STN Express query preparation.

=> S L4

SAMPLE SEARCH INITIATED 13:19:11 FILE 'CASREACT'

SCREENING COMPLETE - 32435 REACTIONS TO VERIFY FROM 2602 DOCUMENTS

15.4% DONE 5000 VERIFIED 188 HIT RXNS (4 INCOMP) 11 DOCS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.08

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 638192 TO 659208
PROJECTED ANSWERS: 1581 TO 2839

L5 11 SEA SSS SAM L4 (188 REACTIONS)

=> s l5 full

FULL SEARCH INITIATED 13:19:29 FILE 'CASREACT'

SCREENING

SCREENING

SCREENING COMPLETE - 647040 REACTIONS TO VERIFY FROM 51482 DOCUMENTS

34.9% DONE 225500 VERIFIED 5730 HIT RXNS (368 INCOMP) 943 DOCS

61.1% DONE 395246 VERIFIED 10586 HIT RXNS (1110 INCOMP) 1465 DOCS

100.0% DONE 647040 VERIFIED 16702 HIT RXNS (1627 INCOMP) 2229 DOCS

SEARCH TIME: 00.01.25

L6 2229 SEA SSS FUL L4 (16702 REACTIONS)

=> s l4 full

FULL SEARCH INITIATED 13:21:06 FILE 'CASREACT'

SCREENING

SCREENING

SCREENING COMPLETE - 647040 REACTIONS TO VERIFY FROM 51482 DOCUMENTS

54.0% DONE 349335 VERIFIED 9370 HIT RXNS (1022 INCOMP) 1317 DOCS

94.9% DONE 614103 VERIFIED 15752 HIT RXNS (1536 INCOMP) 2116 DOCS

100.0% DONE 647040 VERIFIED 16702 HIT RXNS (1627 INCOMP) 2229 DOCS

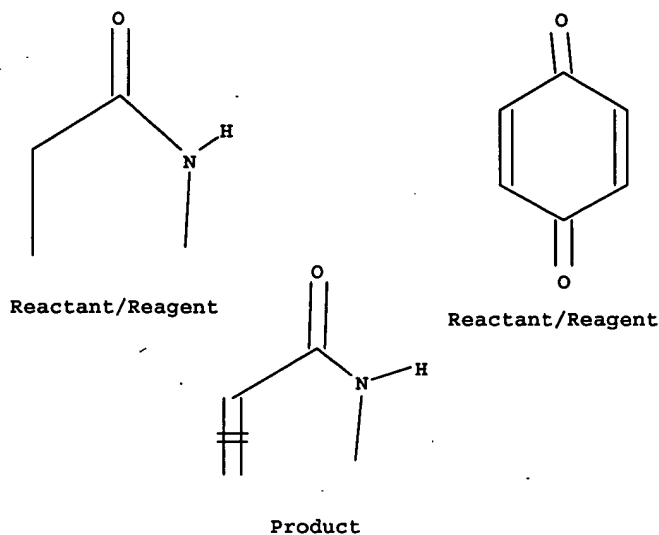
Print selected from 10565446_Rxn2.trn

SEARCH TIME: 00.01.16

L7 2229 SEA SSS FUL L4 (16702 REACTIONS)

Structure task started on Sat Jan 20, 2007 at 11:54 AM

SEARCH for substructures of more complex structures
Explored Reactions containing Reaction Structure in CASREACT.
Input structure:



137 Reactions

Kept records: 30.

Copyrights:

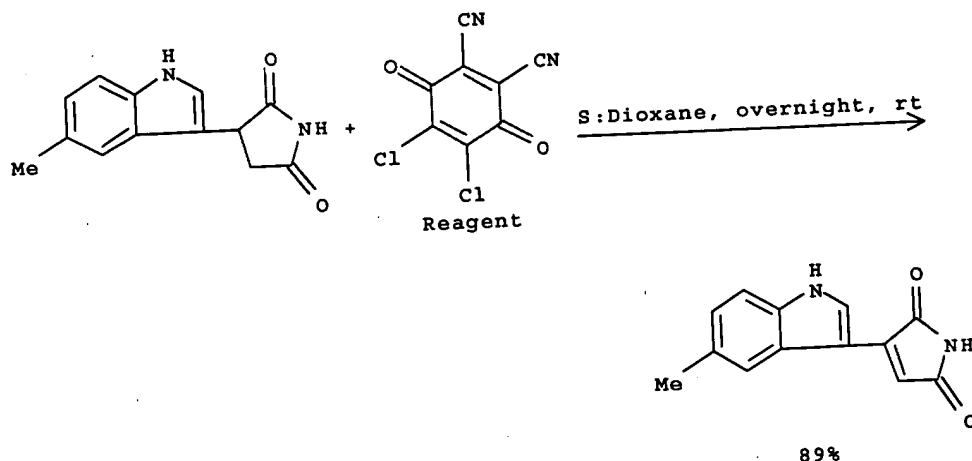
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REGISTRY: Copyright © 2006 American Chemical Society. All Rights Reserved. (Some records contain information from GenBank(R). See also: Benson D.A., Karsch-Mizrachi I., Lipman D.J., Ostell J., Rapp B.A., Wheeler D.L. Genbank. Nucl. Acids Res. 28(1):15-18 (2000). Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.)

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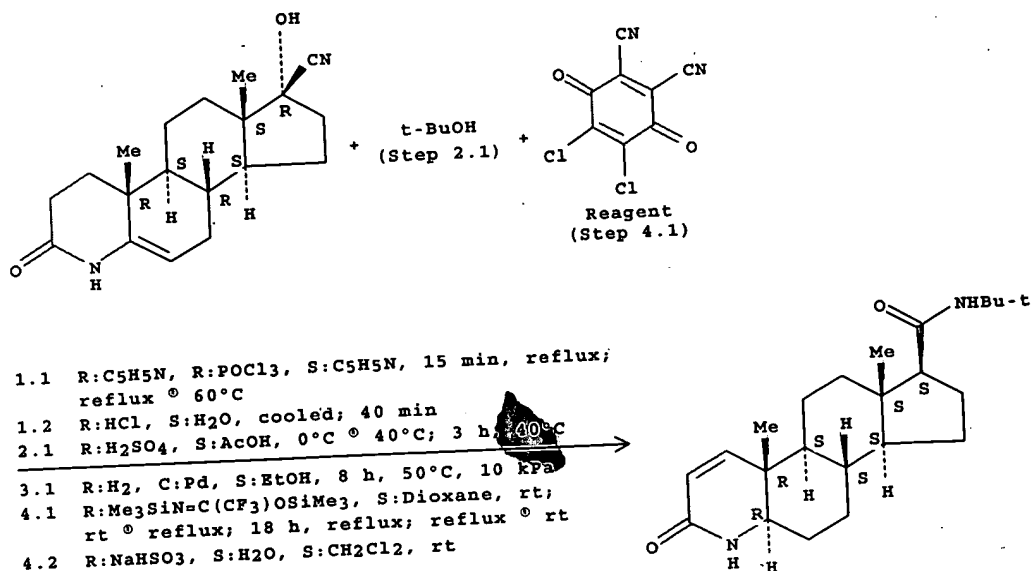


NOTE: Reactants: 1, Reagents: 1, Solvents: 1,
Steps: 1, Stages: 1

Bioorganic & Medicinal Chemistry, 14(11), 3825-3834; 2006

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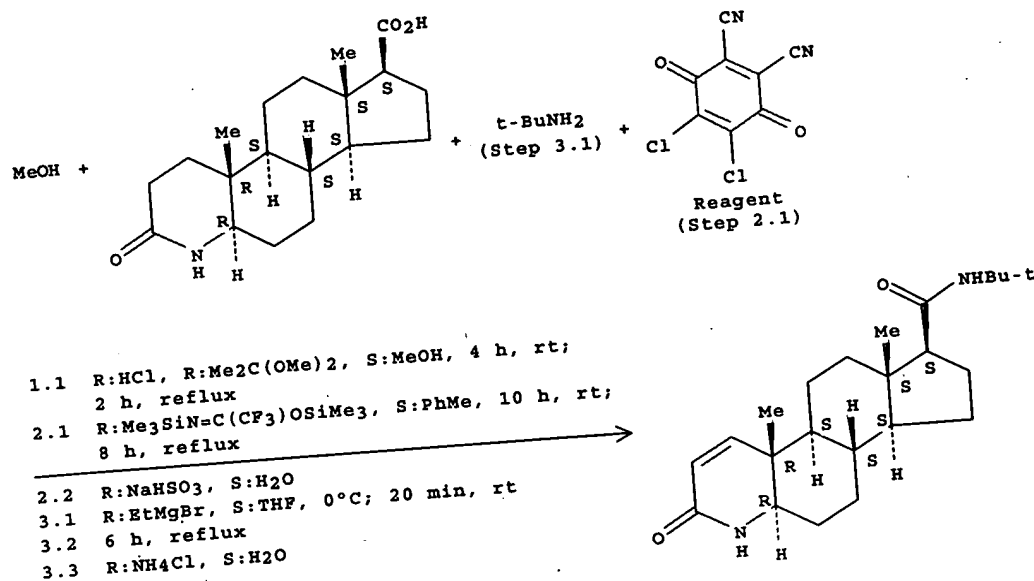
NOTE: 3) stereoselective,
Reactants: 2, Reagents: 8, Catalysts: 1, Solvents: 6,
Steps: 4, Stages: 6, Most stages in any one step: 2

Steroids, 70(10), 690-693; 2005

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derived from the following sources: ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.)

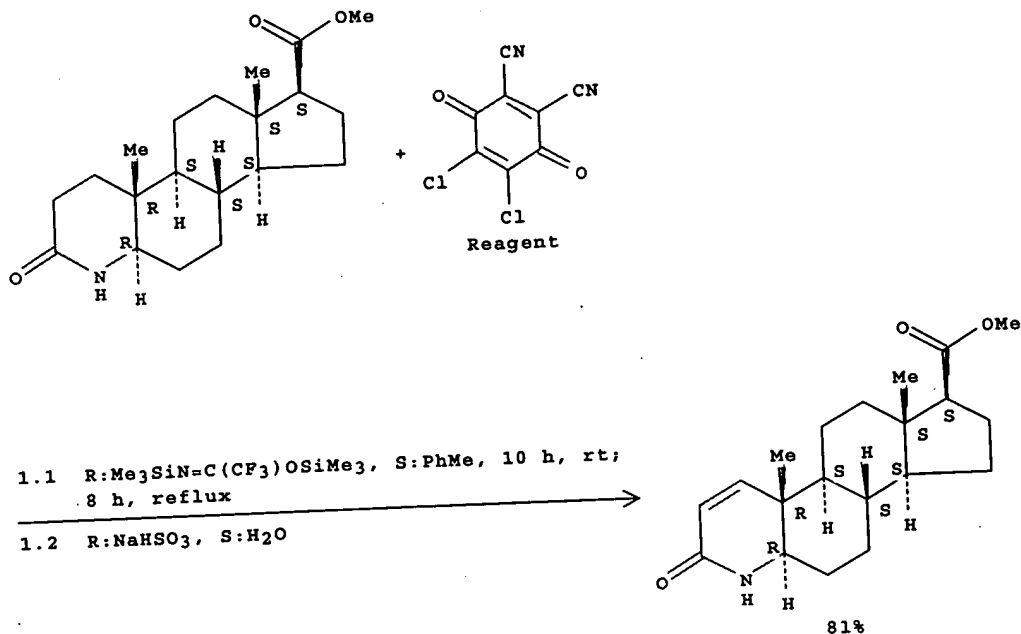


NOTE: 3) Grignard reaction,
Reactants: 3, Reagents: 7, Solvents: 4,
Steps: 3, Stages: 6, Most stages in any one step: 3

Zhongguo Yaoxue Zazhi (Beijing, China), 39(3), 226-228; 2004

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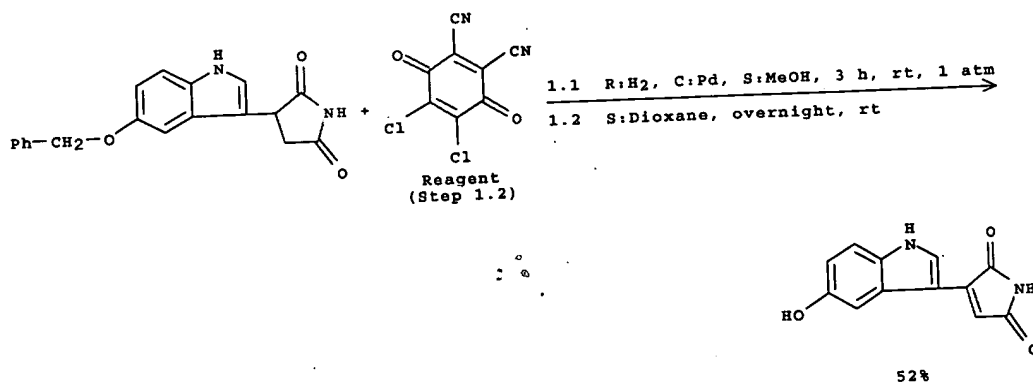


NOTE: Reactants: 1, Reagents: 3, Solvents: 2,
Steps: 1, Stages: 2

Zhongguo Yaoxue Zazhi (Beijing, China), 39(3), 226-228; 2004

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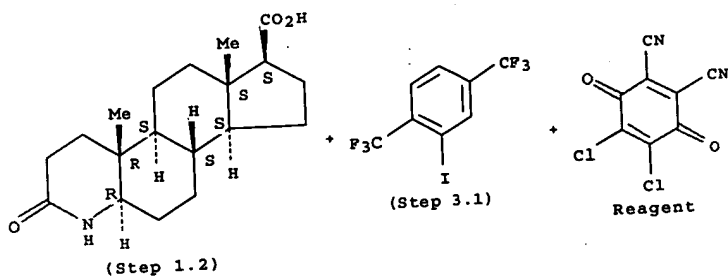
NOTE: Reactants: 1, Reagents: 2, Catalysts: 1, Solvents: 2,
Steps: 1, Stages: 2

Tetrahedron, 61(23), 5599-5614; 2005

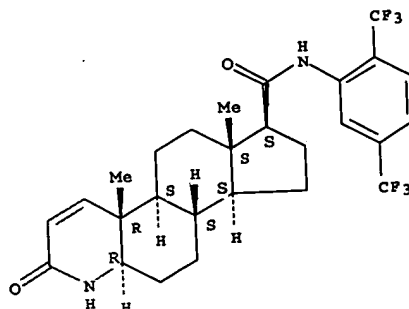
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Kieslich.)



- 1.1 S:PhMe, 2 h, reflux; reflux @ 35°C
- 1.2 R:F₃CC(=O)NH₂, R:CF₃SO₃H, 25-35°C;
20-24 h, 35°C @ 108°C; 108°C @ 60°C
- 1.3 S:H₂O
- 2.1 S:PhMe, 0.5-1 h, reflux
- 2.2 R:C₅H₅N, reflux @ 35°C; 0.25 h
- 2.3 R:SOCl₂, 0.33 h; 2-3 h, 25-35°C
- 2.4 R:NH₃, 8-10 h
- 3.1 R:K₂CO₃, R:Cu, S:Xylene; 50-60 h, 140-150°C;
150°C @ 35°C; 3-4 h, 25-35°C

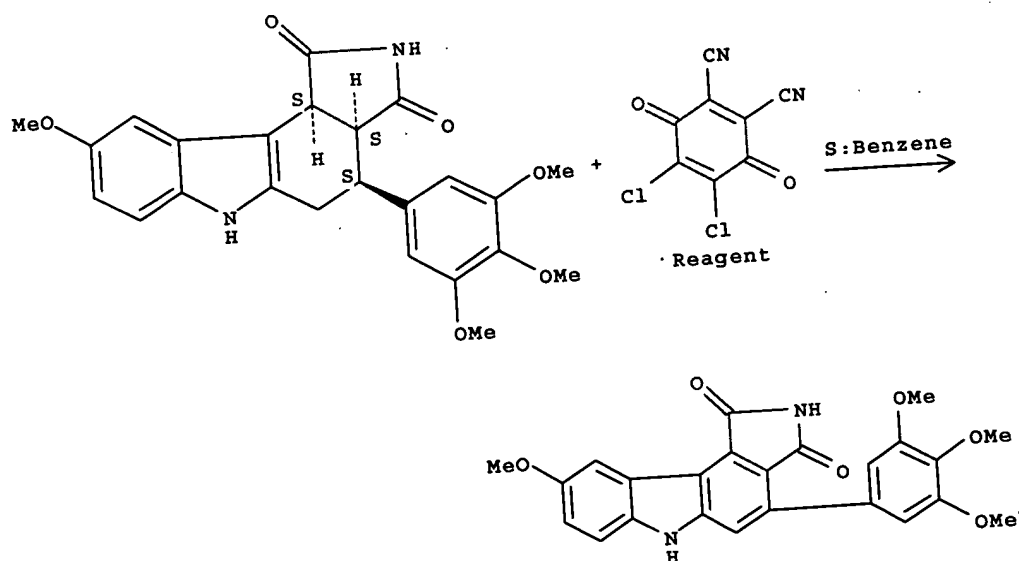


NOTE: 1) workup, 3) thermal, workup,
Reactants: 2, Reagents: 8, Solvents: 3,
Steps: 3, Stages: 8, Most stages in any one step: 4

U.S. Pat. Appl. Publ., 2005059692, 17 Mar 2005

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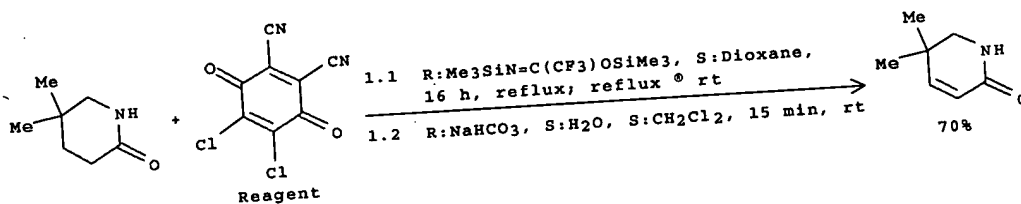


NOTE: Reactants: 1, Reagents: 1, Solvents: 1,
Steps: 1, Stages: 1

Bioorganic & Medicinal Chemistry, 11(16), 3413-3421; 2003

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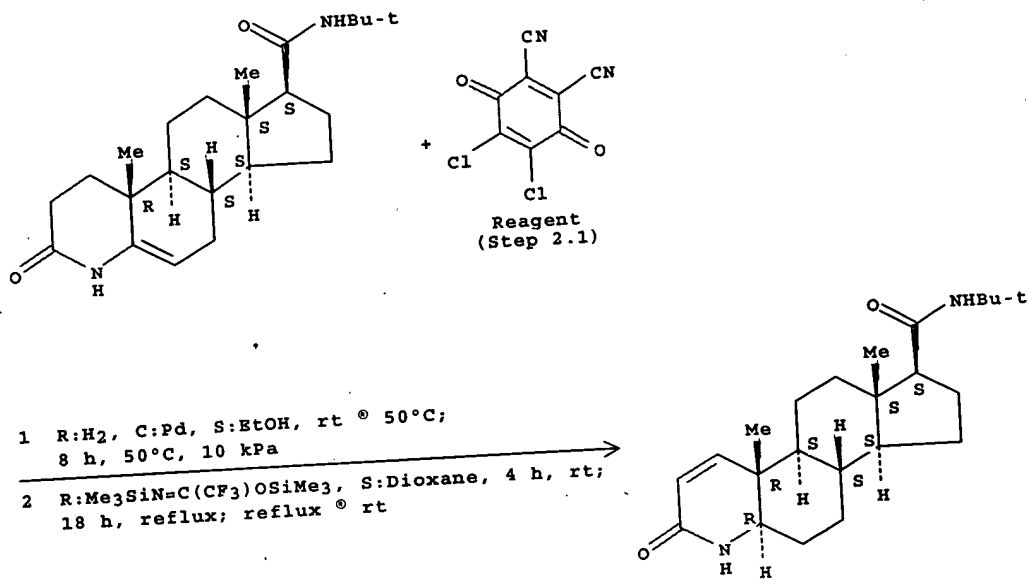


NOTE: Reactants: 1, Reagents: 3, Solvents: 3,
Steps: 1, Stages: 2

Bioorganic & Medicinal Chemistry, 11(5), 689-702; 2003

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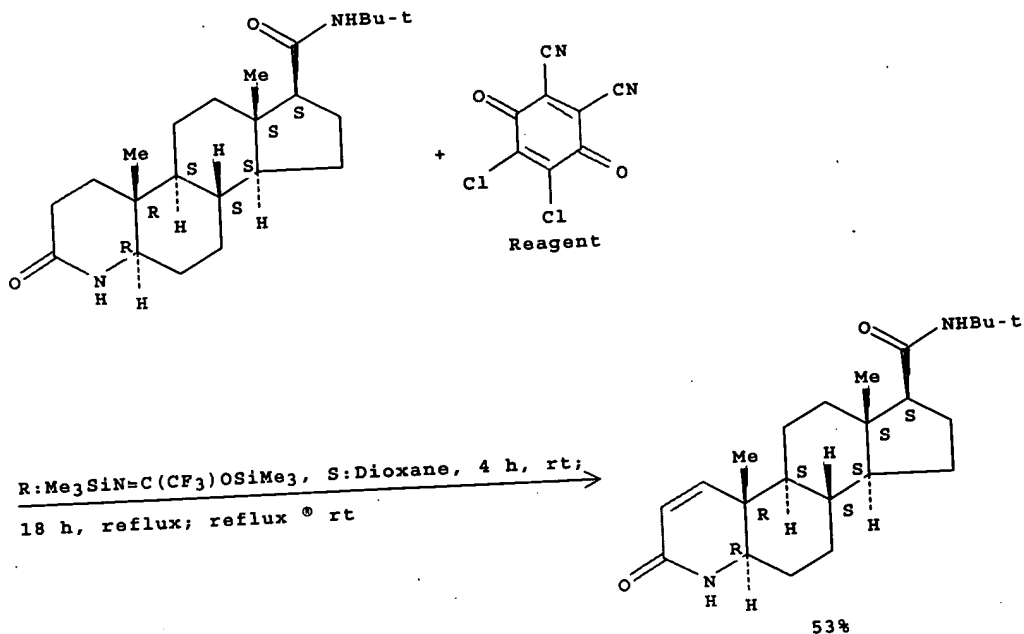


NOTE: 1) stereoselective,
Reactants: 1, Reagents: 3, Catalysts: 1, Solvents: 2,
Steps: 2, Stages: 2, Most stages in any one step: 1

Xiangtan Daxue Ziran Kexue Xuebao, 25(2), 43-45; 2003

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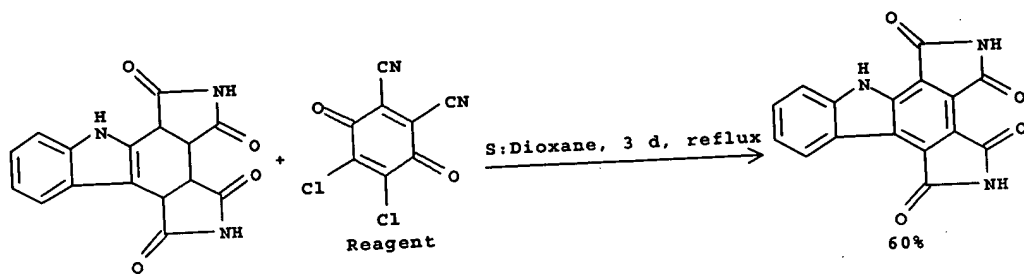


NOTE: Reactants: 1, Reagents: 2, Solvents: 1,
Steps: 1, Stages: 1

Xiangtan Daxue Ziran Kexue Xuebao, 25(2), 43-45; 2003

CASREACT

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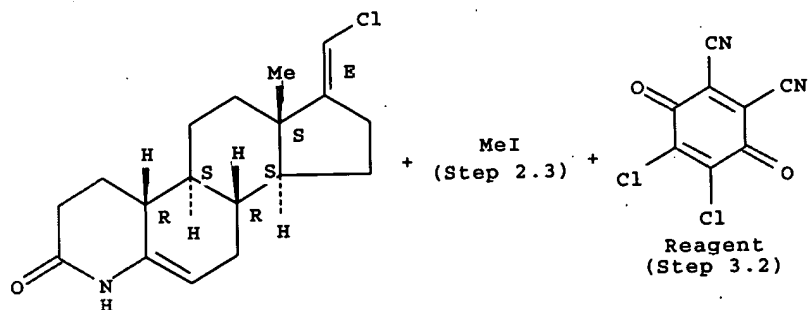


NOTE: Reactants: 1, Reagents: 1, Solvents: 1,
Steps: 1, Stages: 1

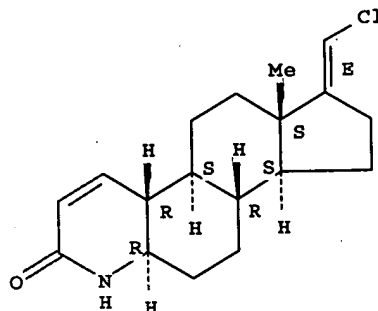
Tetrahedron Letters, 44(20), 3935-3937; 2003

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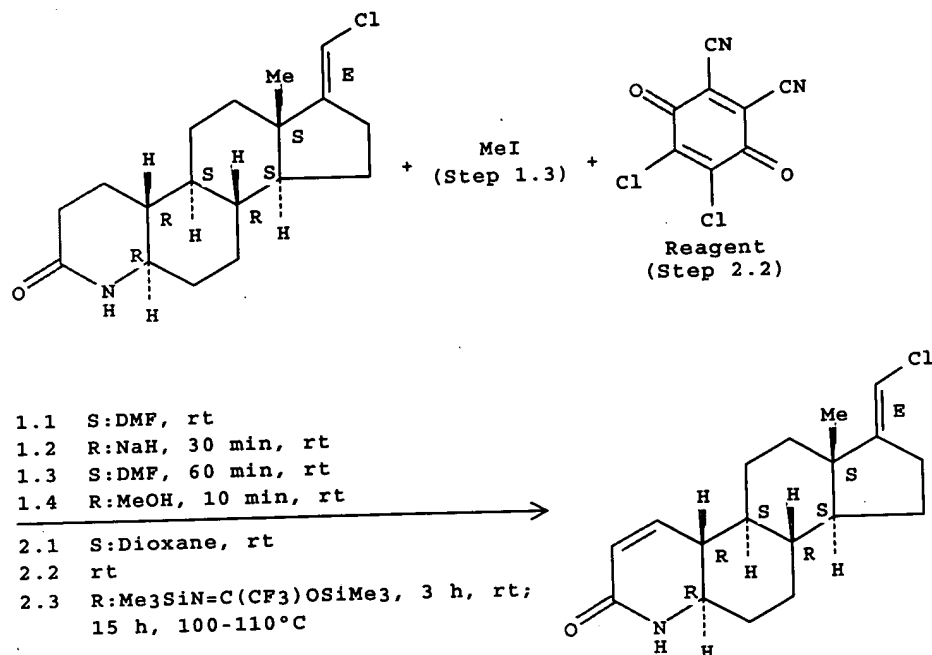
- 1.1 S:DMF, rt
 1.2 R:HCO₂H, rt
 1.3 R:K₂CO₃, rt; 12 h, reflux
 2.1 S:DMF, rt
 2.2 R:NaH, 30 min, rt
 2.3 S:DMF, 60 min, rt
 2.4 R:MeOH, 10 min, rt
 3.1 S:Dioxane, rt
 3.2 rt
 3.3 R:Me₃SiN=C(CF₃)OSiMe₃, 3 h, rt;
 15 h, 100-110°C



NOTE: Reactants: 2, Reagents: 6, Solvents: 2,
 Steps: 3, Stages: 10, Most stages in any one step: 4

PCT Int. Appl., 2003020744, 13 Mar 2003
 CASREACT

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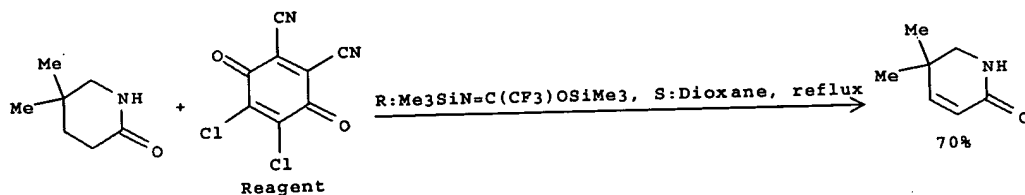


NOTE: Reactants: 2, Reagents: 4, Solvents: 2,
 Steps: 2, Stages: 7, Most stages in any one step: 4

PCT Int. Appl., 2003020744, 13 Mar 2003

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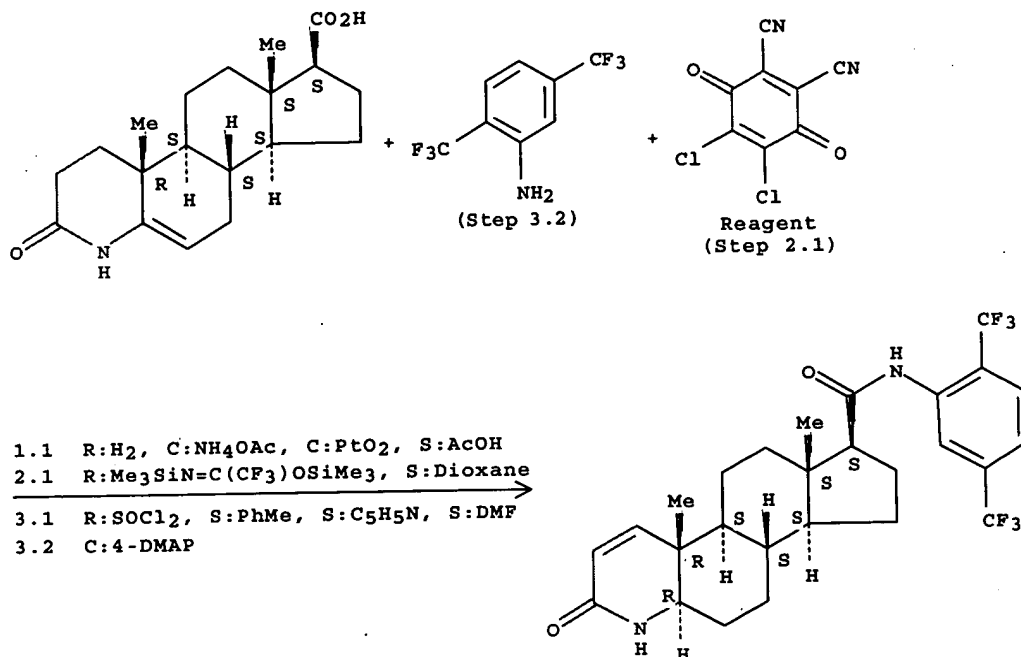


NOTE: Reactants: 1, Reagents: 2, Solvents: 1,
 Steps: 1, Stages: 1

Bioorganic & Medicinal Chemistry Letters, 12(17), 2291-2294; 2002

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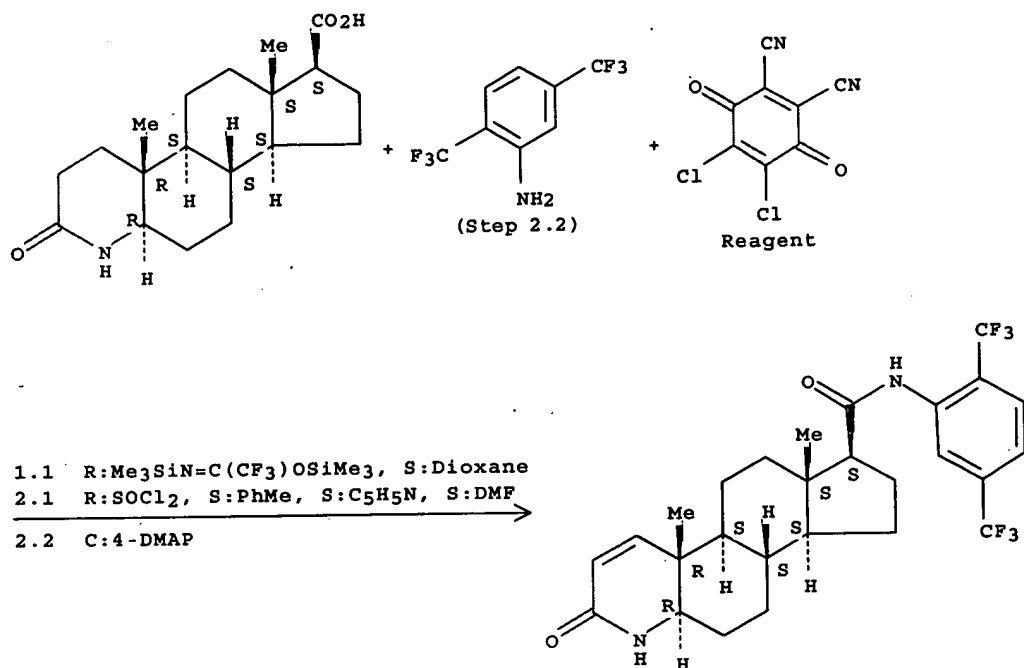


NOTE: 1) stereoselective,
 Reactants: 2, Reagents: 4, Catalysts: 3, Solvents: 5,
 Steps: 3, Stages: 4, Most stages in any one step: 2

PCT Int. Appl., 2002046207, 13 Jun 2002

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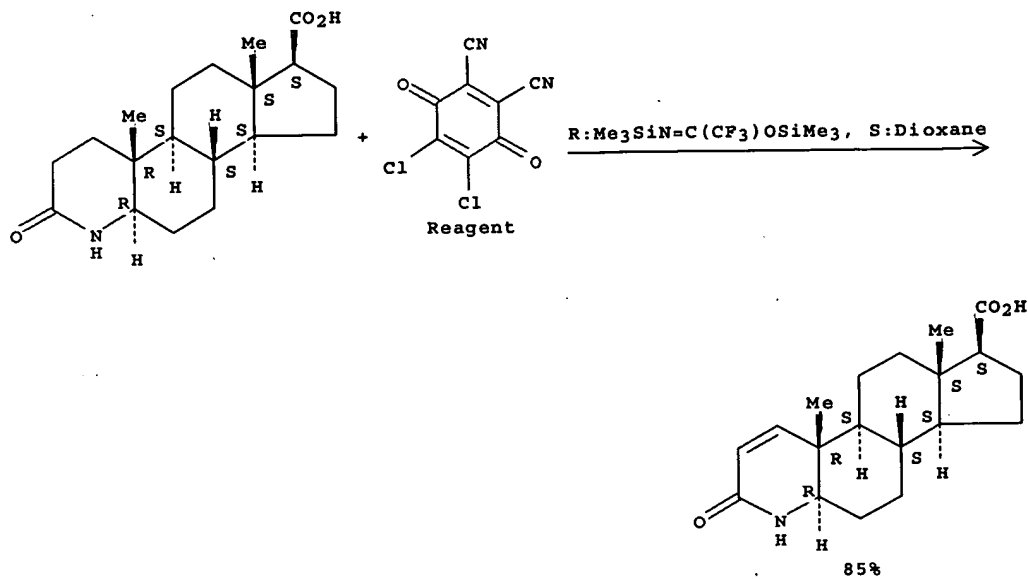


NOTE: Reactants: 2, Reagents: 3, Catalysts: 1, Solvents: 4,
 Steps: 2, Stages: 3, Most stages in any one step: 2

PCT Int. Appl., 2002046207, 13 Jun 2002

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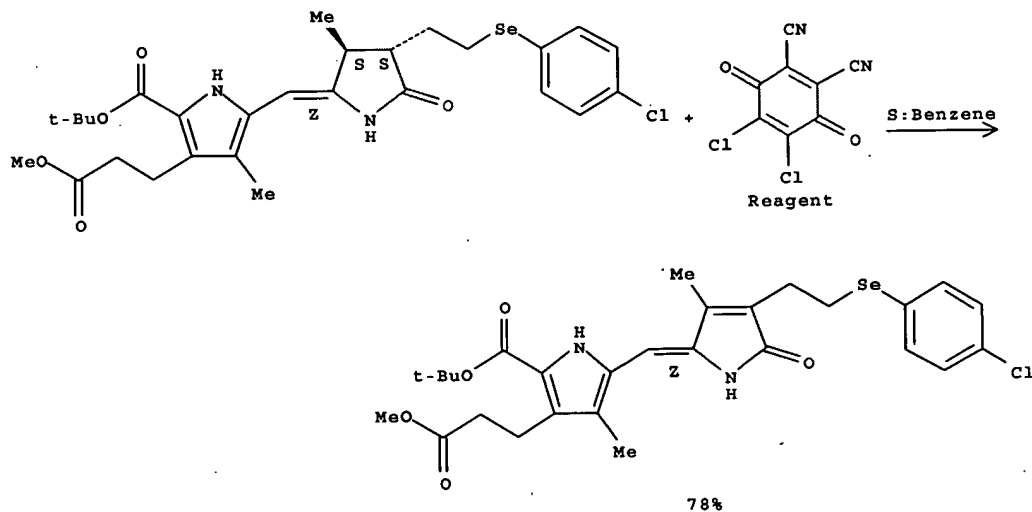


NOTE: Reactants: 1, Reagents: 2, Solvents: 1,
Steps: 1, Stages: 1

PCT Int. Appl., 2002046207, 13 Jun 2002

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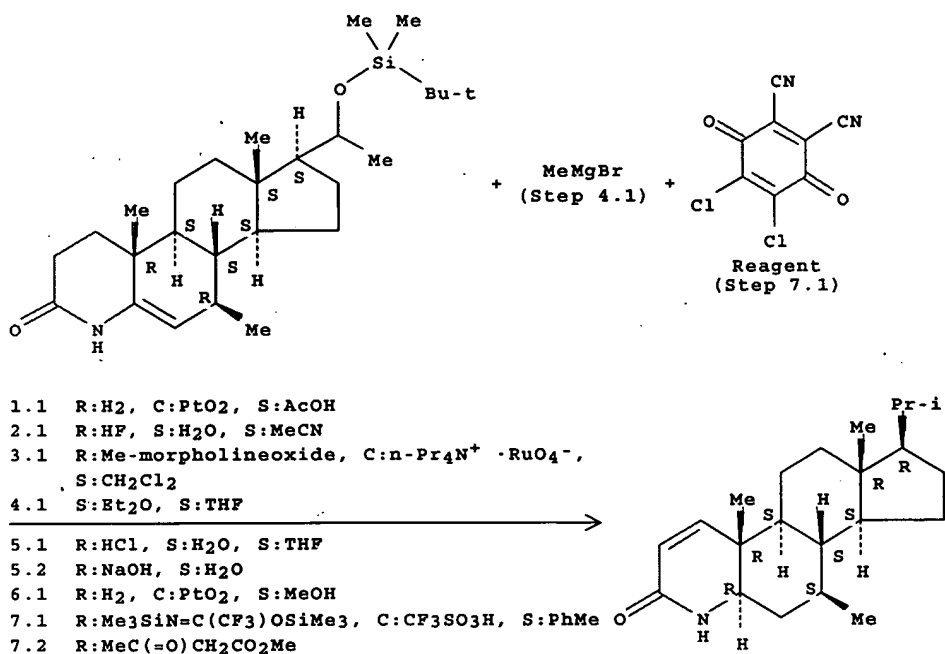
NOTE: Reactants: 1, Reagents: 1, Solvents: 1,
Steps: 1, Stages: 1

Journal of Organic Chemistry, 65(25), 8478-8489; 2000

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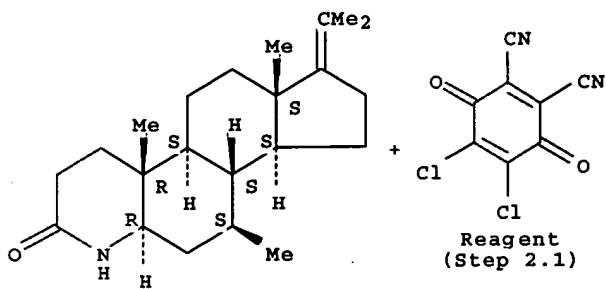


NOTE: 1) stereoselective, 3) regioselective; 4A mol. sieves, 4) key step, 6) stereoselective,
 Reactants: 2, Reagents: 8, Catalysts: 3, Solvents: 8,
 Steps: 7, Stages: 9, Most stages in any one step: 2

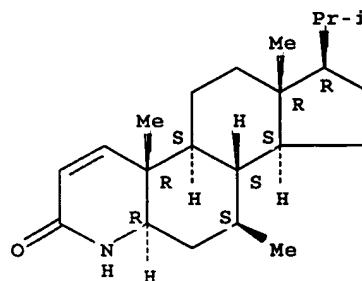
U.S., 5763361, 09 Jun 1998

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1.1 R:H₂, C:PtO₂, S:MeOH
 2.1 R:Me₃SiN=C(CF₃)OSiMe₃, C:CF₃SO₃H, S:PhMe
 2.2 R:MeC(=O)CH₂CO₂Me

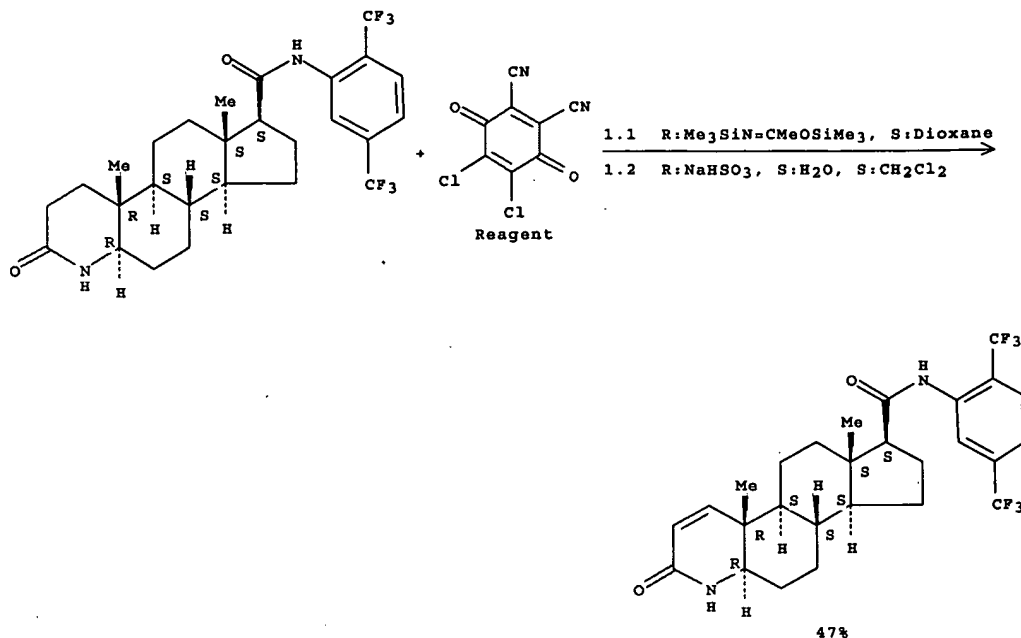


NOTE: 1) stereoselective,
 Reactants: 1, Reagents: 4, Catalysts: 2, Solvents: 2,
 Steps: 2, Stages: 3, Most stages in any one step: 2

U.S., 5763361, 09 Jun 1998

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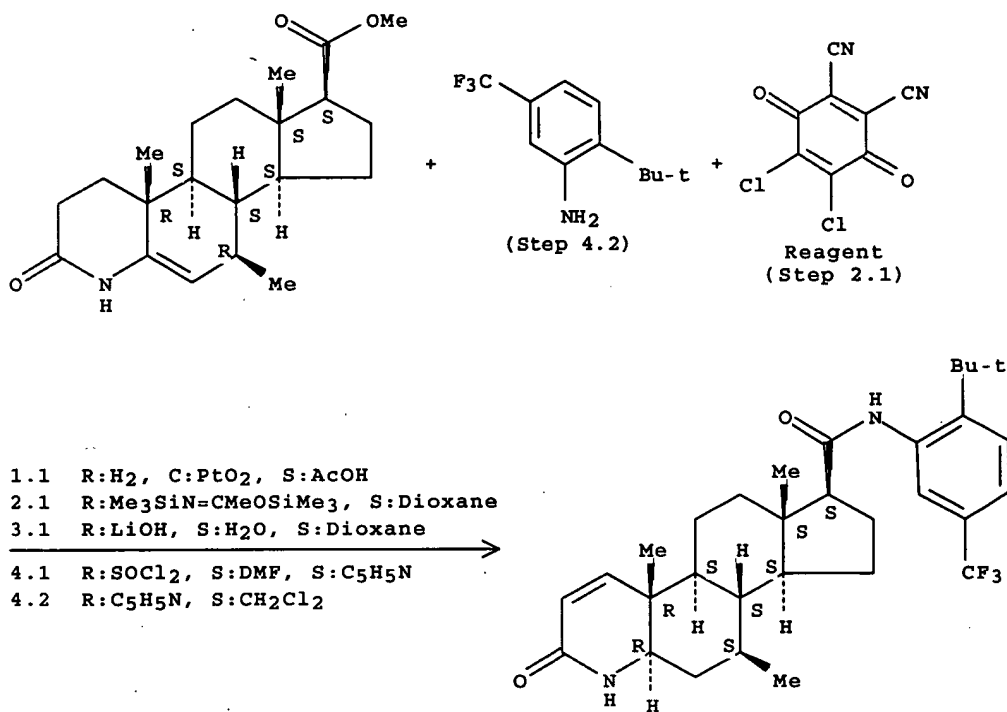


NOTE: Reactants: 1, Reagents: 3, Solvents: 3,
Steps: 1, Stages: 2

PCT Int. Appl., 9507927, 23 Mar 1995

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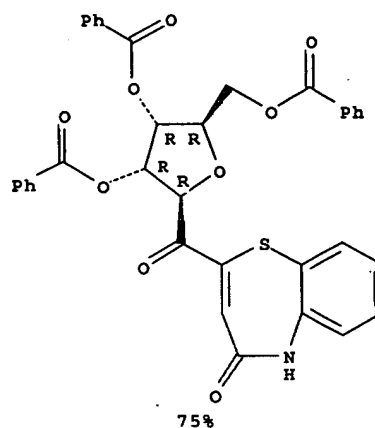
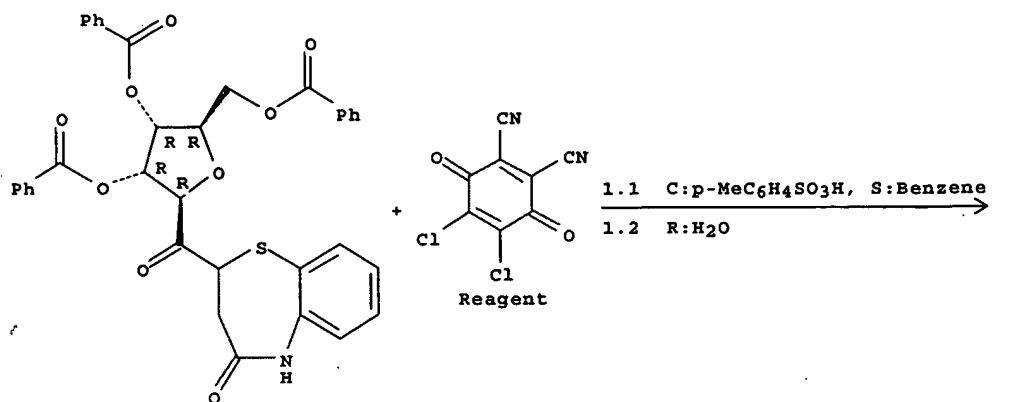


NOTE: Reactants: 2, Reagents: 6, Catalysts: 1, Solvents: 6,
 Steps: 4, Stages: 5, Most stages in any one step: 2

PCT Int. Appl., 9507926, 23 Mar 1995

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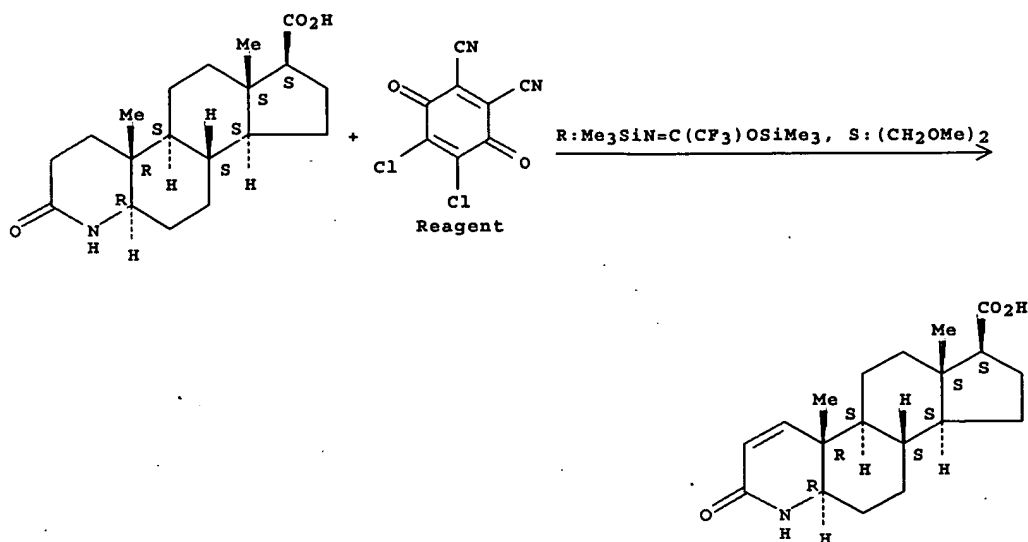


NOTE: Reactants: 1, Reagents: 2, Catalysts: 1, Solvents: 1,
Steps: 1, Stages: 2

Heterocycles, 34(11), 2131-6; 1992

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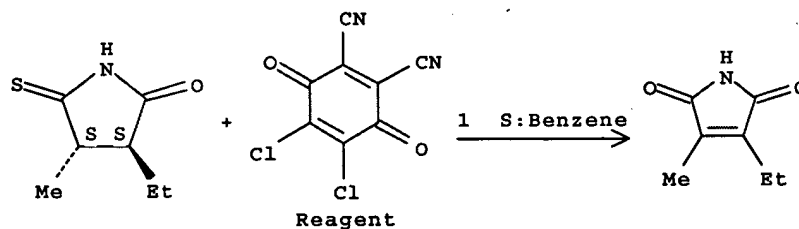


NOTE: Thermal,
 Reactants: 1, Reagents: 2, Solvents: 1,
 Steps: 1, Stages: 1

U.S., 5084574, 28 Jan 1992

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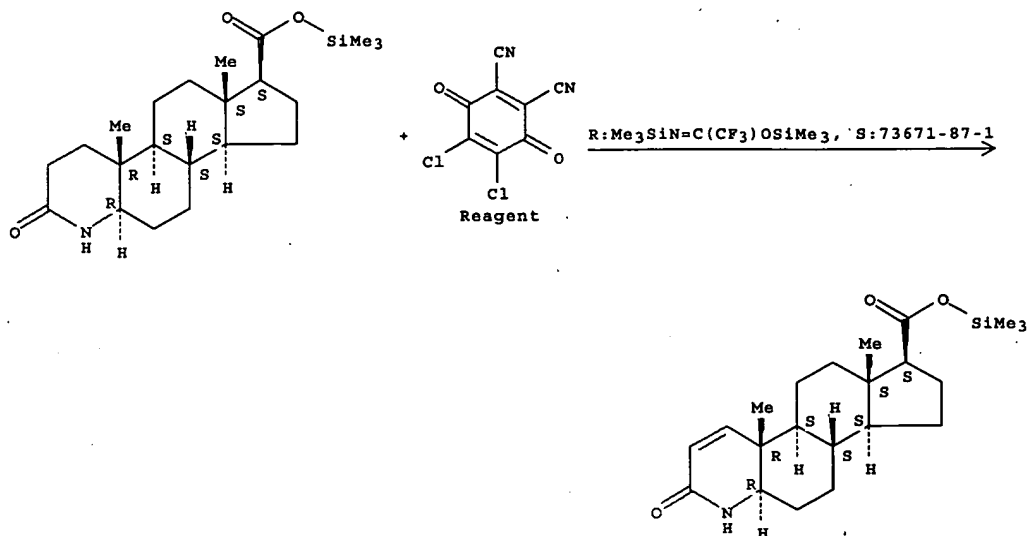


NOTE: Reactants: 1, Reagents: 1, Solvents: 1,
 Steps: 2, Stages: 2, Most stages in any one step: 1

Journal of Organic Chemistry, 54(8), 1876-83; 1989

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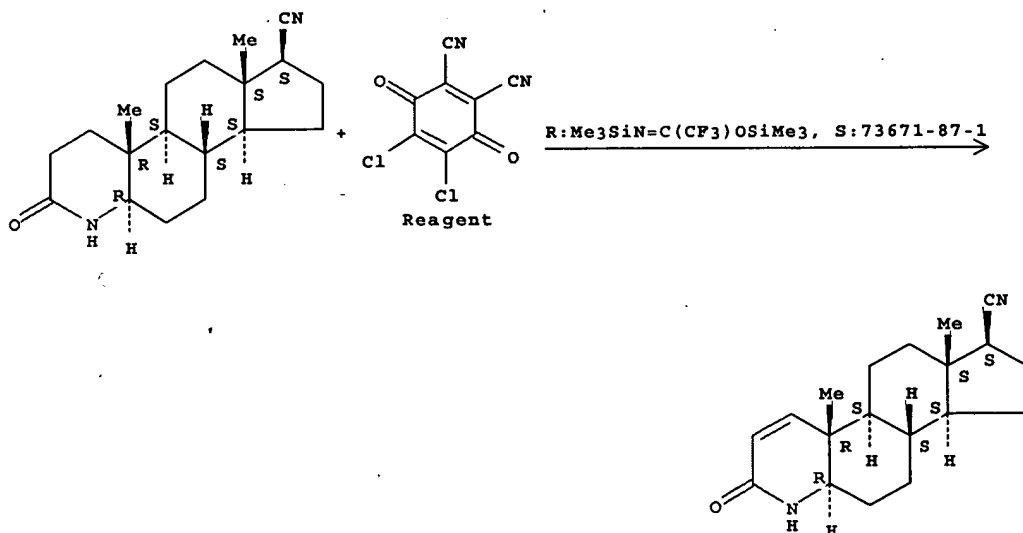


NOTE: Reactants: 1, Reagents: 2, Solvents: 1,
Steps: 1, Stages: 1

Journal of the American Chemical Society, 110(10), 3318-19; 1988

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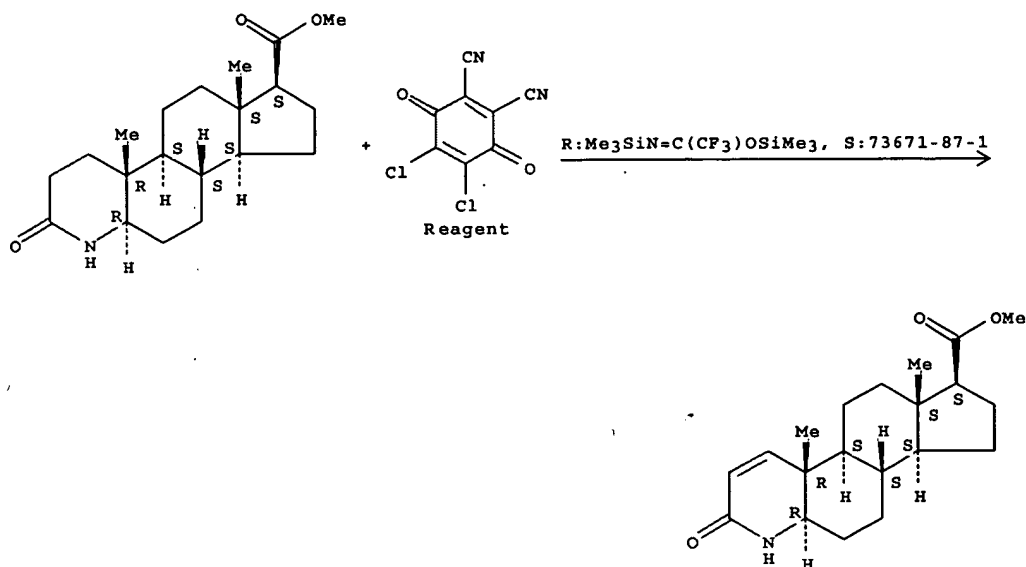
NOTE: Reactants: 1, Reagents: 2, Solvents: 1,
Steps: 1, Stages: 1

Journal of the American Chemical Society, 110(10), 3318-19; 1988

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prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.)

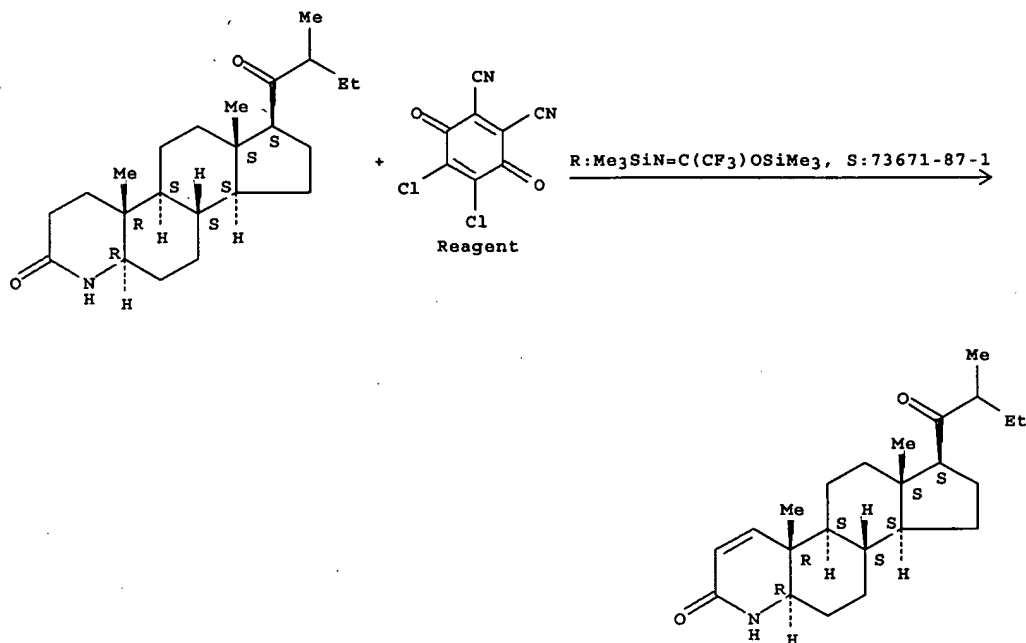


NOTE: Reactants: 1, Reagents: 2, Solvents: 1,
Steps: 1, Stages: 1

Journal of the American Chemical Society, 110(10), 3318-19; 1988

CASREACT

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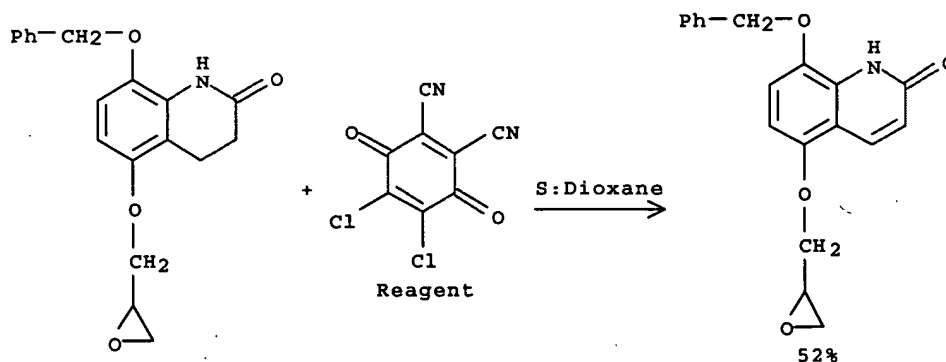


NOTE: Reactants: 1, Reagents: 2, Solvents: 1,
Steps: 1, Stages: 1

Journal of the American Chemical Society, 110(10), 3318-19; 1988

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NOTE: Reactants: 1, Reagents: 1, Solvents: 1,
Steps: 1, Stages: 1

Chemical & Pharmaceutical Bulletin, 35(9), 3699-704; 1987

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